



Sample name: **M12_octanol** Experiment start time: **3/3/2018 7:38:51 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-03015** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

pH-metric Result

logP (XH +) 0.40 ±0.06 (n=50)
logP (neutral X) 3.80 ±0.01 (n=50)

18C-03015 Points 1 to 18

M12_octanol concentration factor 1.084
Carbonate 0.0827 mM
Acidity error -3.00593 mM

18C-03015 Points 19 to 29

M12_octanol concentration factor 1.664
Carbonate 0.1338 mM
Acidity error -2.74094 mM

18C-03015 Points 30 to 56

M12_octanol concentration factor 0.918
Carbonate 0.0569 mM
Acidity error 8.57201 mM

Warnings and errors

Errors None
Warnings None

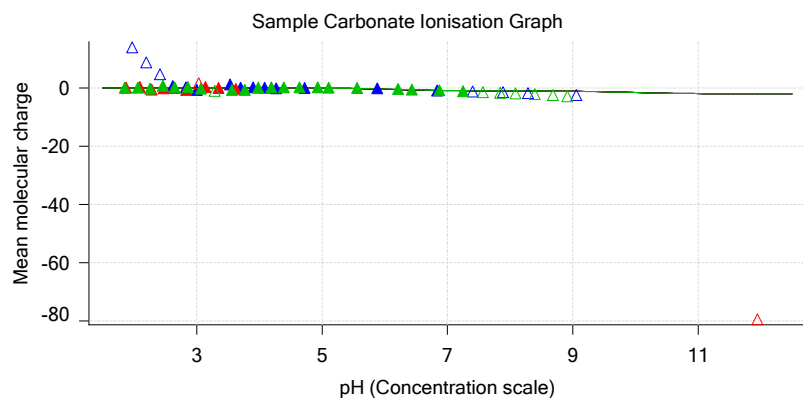
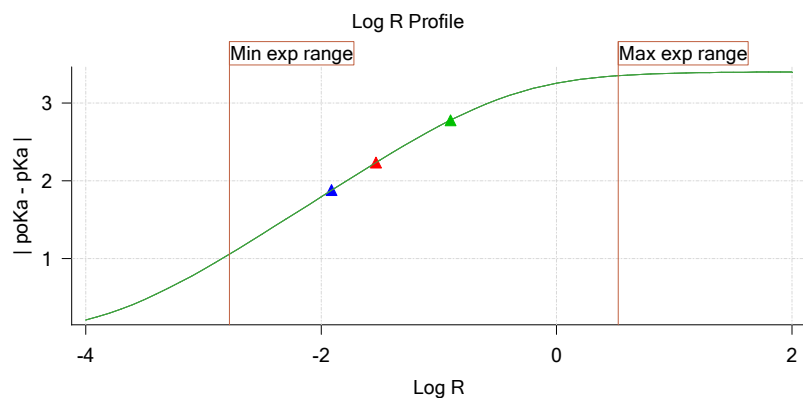
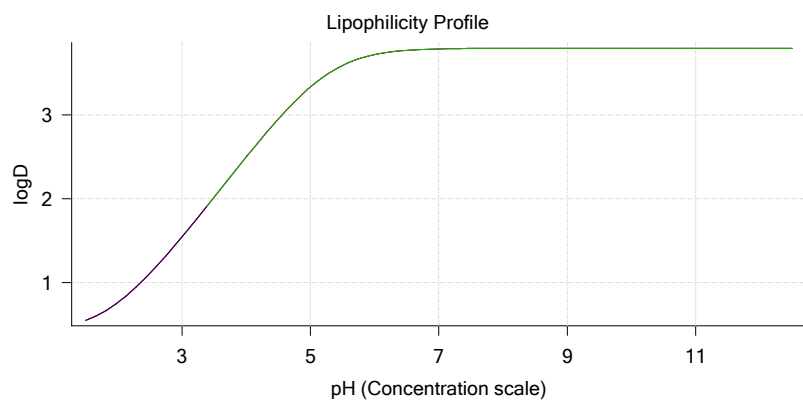
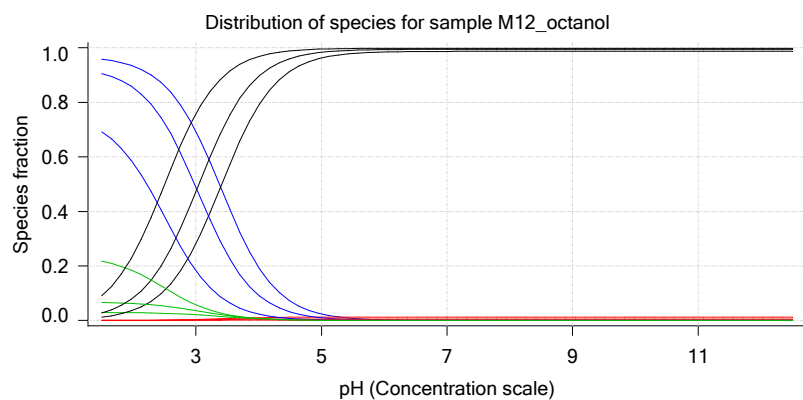
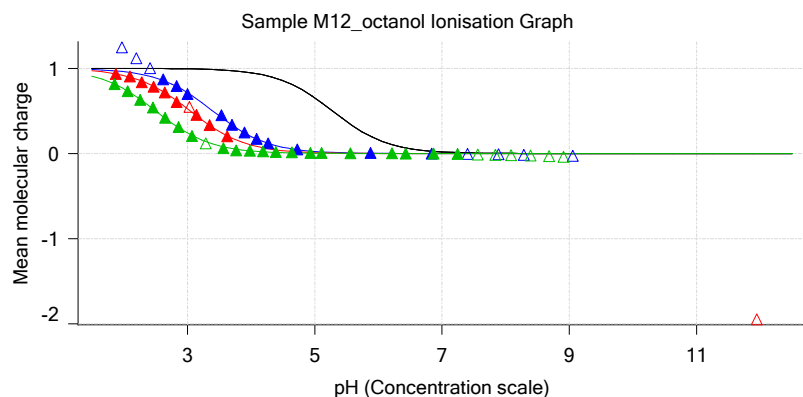
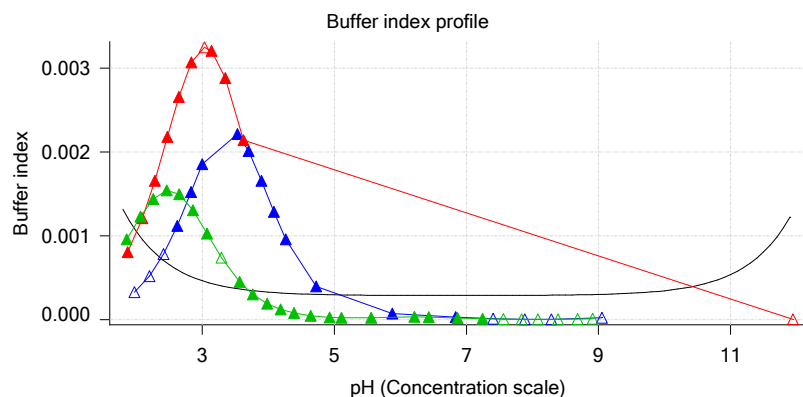
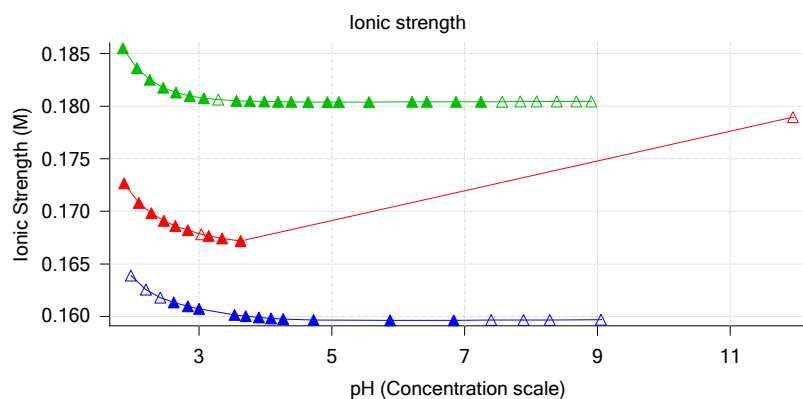
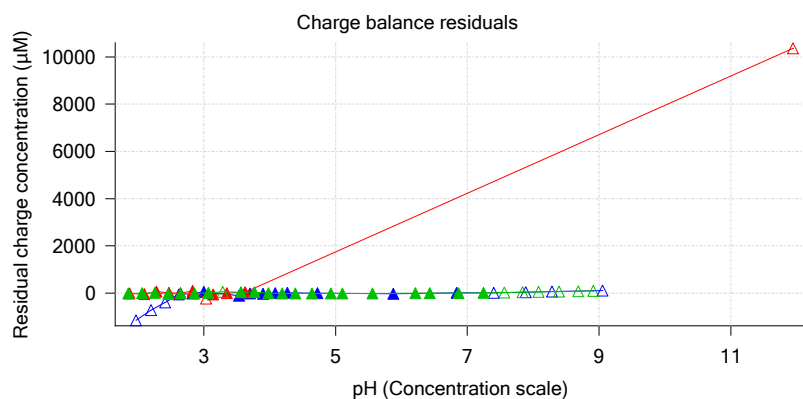
Sample logD and percent species

pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	0.45	26.11 %	0.00 %	65.29 %	8.60 %	Stomach pH
1.200	0.48	24.86 %	0.00 %	62.16 %	12.97 %	
2.000	0.76	14.72 %	0.01 %	36.81 %	48.46 %	
3.000	1.55	2.75 %	0.01 %	6.86 %	90.38 %	
4.000	2.50	0.30 %	0.02 %	0.75 %	98.93 %	
5.000	3.33	0.03 %	0.02 %	0.08 %	99.88 %	Blood pH
6.000	3.72	0.00 %	0.02 %	0.01 %	99.97 %	
6.500	3.77	0.00 %	0.02 %	0.00 %	99.98 %	
7.000	3.79	0.00 %	0.02 %	0.00 %	99.98 %	
7.400	3.79	0.00 %	0.02 %	0.00 %	99.98 %	
8.000	3.80	0.00 %	0.02 %	0.00 %	99.98 %	
9.000	3.80	0.00 %	0.02 %	0.00 %	99.98 %	
10.000	3.80	0.00 %	0.02 %	0.00 %	99.98 %	
11.000	3.80	0.00 %	0.02 %	0.00 %	99.98 %	
12.000	3.80	0.00 %	0.02 %	0.00 %	99.98 %	

Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

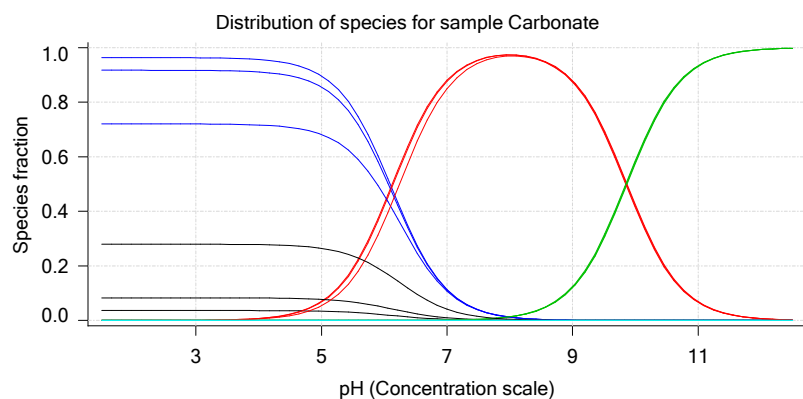
Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Graphs



Sample name:	M12_octanol	Experiment start time:	3/3/2018 7:38:51 PM
Assay name:	pH-metric high logP	Analyst:	Pion
Assay ID:	18C-03015	Instrument ID:	T312060
Filename:	C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r		

Graphs (continued)



Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 1 of 3 18C-03015 Points 1 to 18

Overall results

RMSD 0.115
 Average ionic strength 0.160 M
 Average temperature 24.9°C
 Partition ratio 0.0123 : 1
 Analyte concentration range 3571.6 µM to 3683.7 µM
 Total points considered 11 of 18

Warnings and errors

Errors None
 Warnings Excessive acidity error present

Four-Plus parameters

Alpha 0.111 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 S 0.9988 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 jH 1.0 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 jOH -0.8 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r

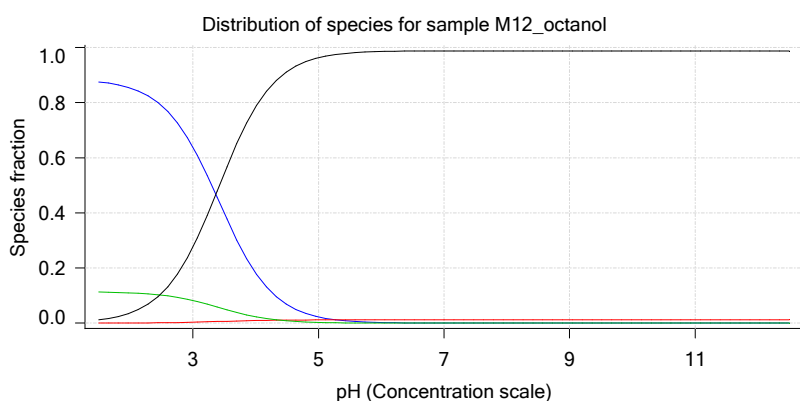
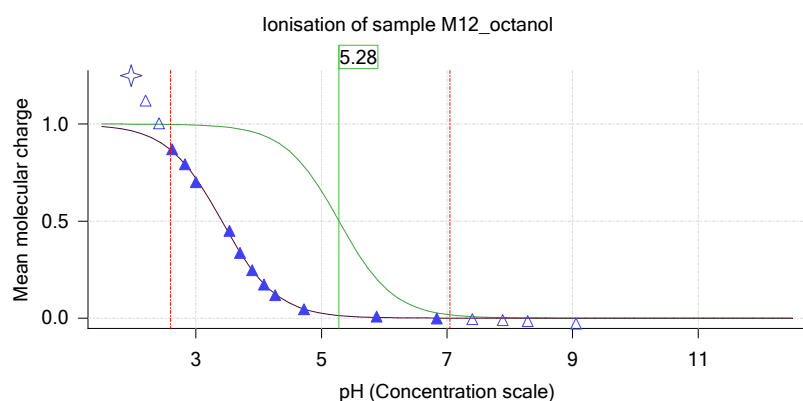
Titrants

0.50 M HCl 0.999058 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 0.50 M KOH 0.999845 3/3/2018 7:38:51 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M12_octanol concentration factor 1.084
 M12_octanol stoichiometry 1.000
 Chloride stoichiometry 1.000
 Base pKa 1 5.28
 logP (XH +) 1.02
 logP (neutral X) 3.82

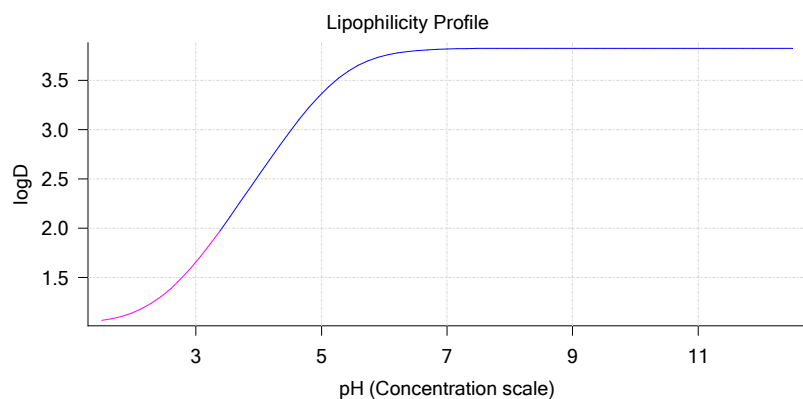
Sample graphs



Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**



Sample graphs (continued)



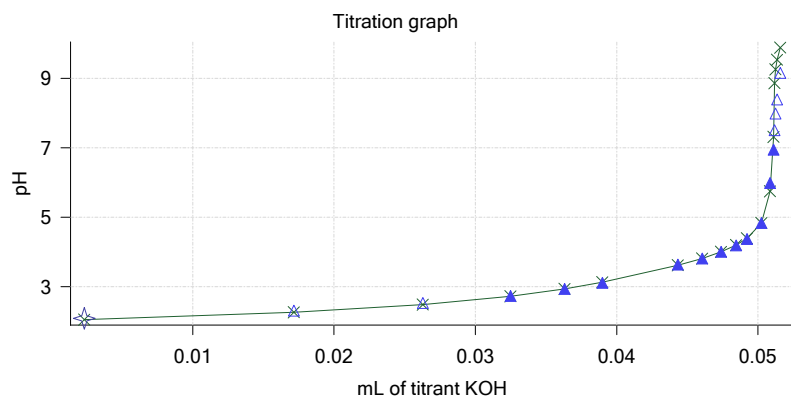
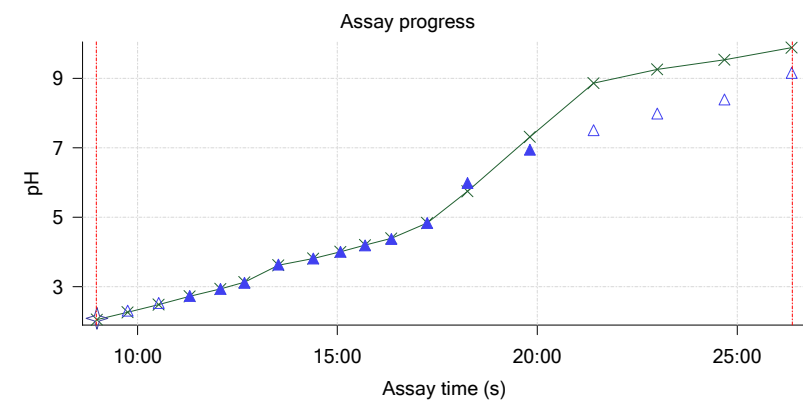
Sample logD and percent species

pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanol	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.03	88.26 %	0.00 %	11.36 %	0.38 %	Stomach pH
1.200	1.04	88.06 %	0.01 %	11.33 %	0.60 %	
2.000	1.15	85.31 %	0.04 %	10.98 %	3.67 %	
3.000	1.66	63.92 %	0.34 %	8.22 %	27.52 %	
4.000	2.54	18.23 %	0.96 %	2.34 %	78.47 %	
5.000	3.36	2.24 %	1.17 %	0.29 %	96.30 %	Blood pH
6.000	3.75	0.23 %	1.20 %	0.03 %	98.54 %	
6.500	3.80	0.07 %	1.20 %	0.01 %	98.71 %	
7.000	3.82	0.02 %	1.20 %	0.00 %	98.77 %	
7.400	3.82	0.01 %	1.20 %	0.00 %	98.79 %	
8.000	3.82	0.00 %	1.20 %	0.00 %	98.79 %	
9.000	3.82	0.00 %	1.20 %	0.00 %	98.80 %	
10.000	3.82	0.00 %	1.20 %	0.00 %	98.80 %	
11.000	3.82	0.00 %	1.20 %	0.00 %	98.80 %	
12.000	3.82	0.00 %	1.20 %	0.00 %	98.80 %	

Carbonate and acidity

 Carbonate 0.083 mM
 Acidity error -3.006 mM

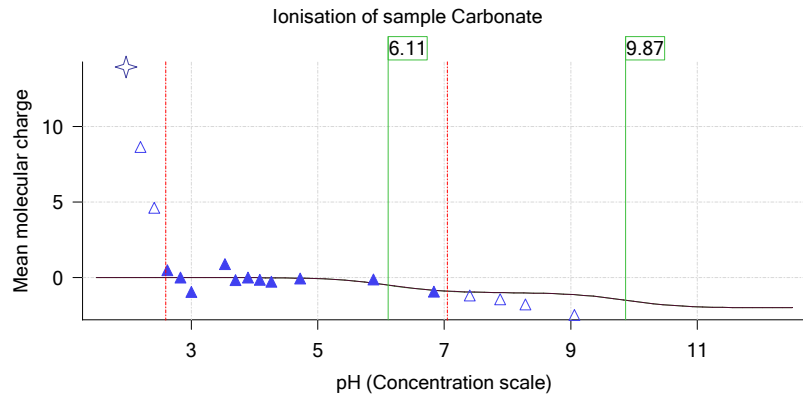
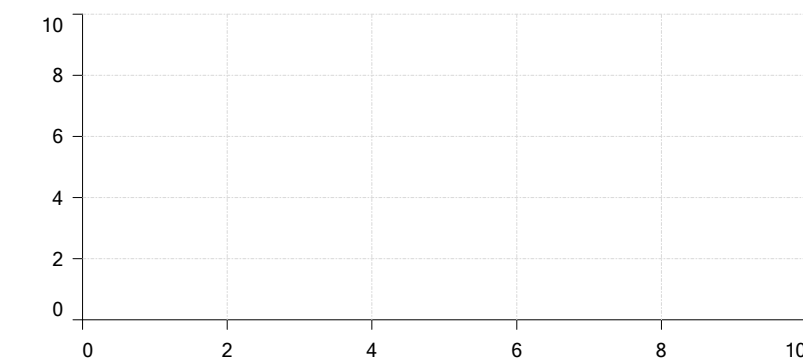
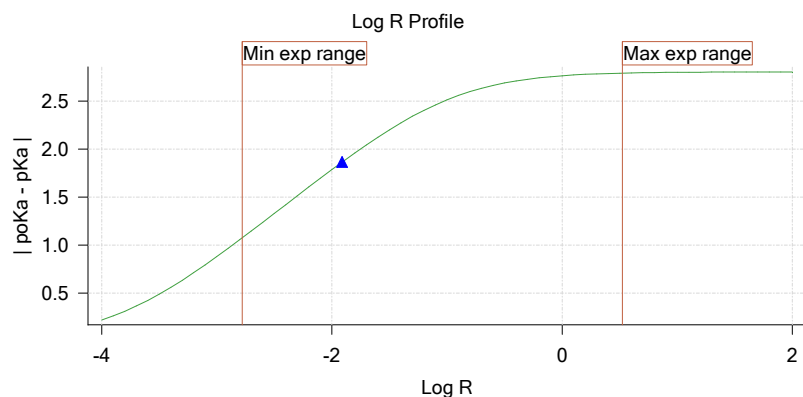
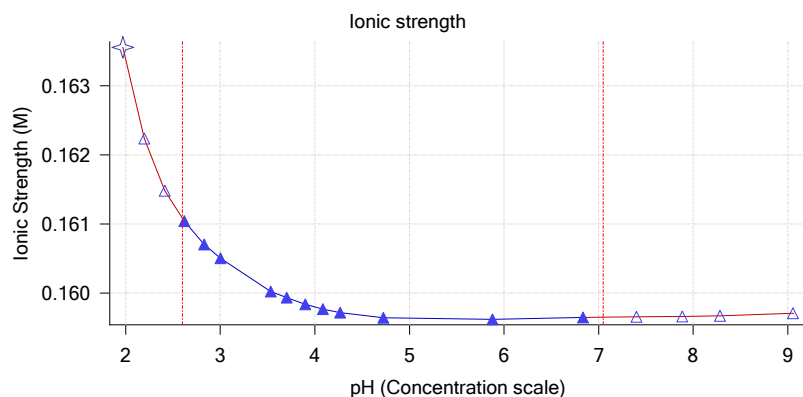
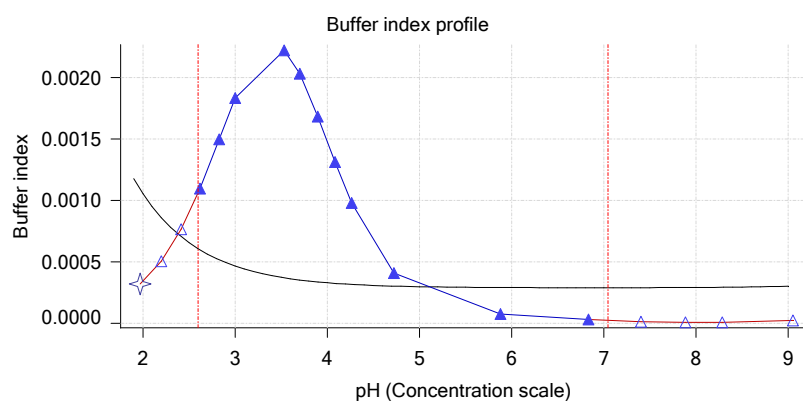
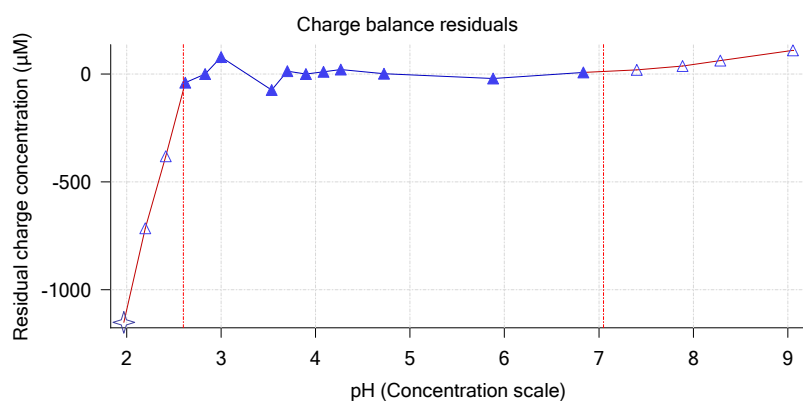
Other graphs



Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

pH-metric high logP Titration 2 of 3 18C-03015 Points 19 to 29

Overall results

RMSD 0.008
 Average ionic strength 0.168 M
 Average temperature 25.0°C
 Partition ratio 0.0293 : 1
 Analyte concentration range 3109.3 µM to 3391.7 µM
 Total points considered 9 of 11

Warnings and errors

Errors None
 Warnings Sample concentration factor out of range
 Excessive acidity error present

Four-Plus parameters

Alpha 0.111 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 S 0.9988 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 jH 1.0 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 jOH -0.8 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r

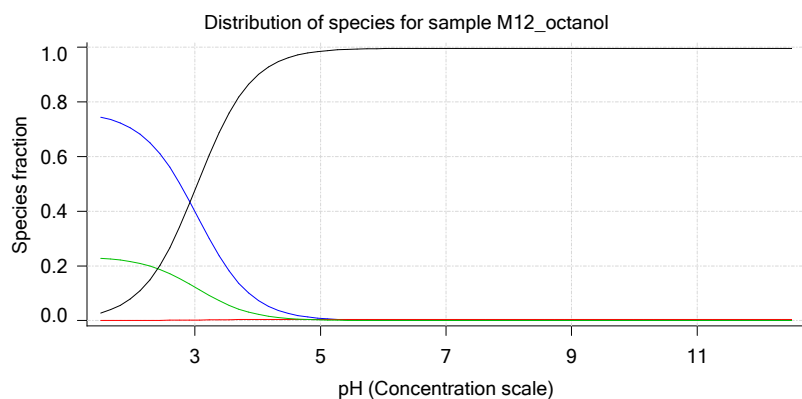
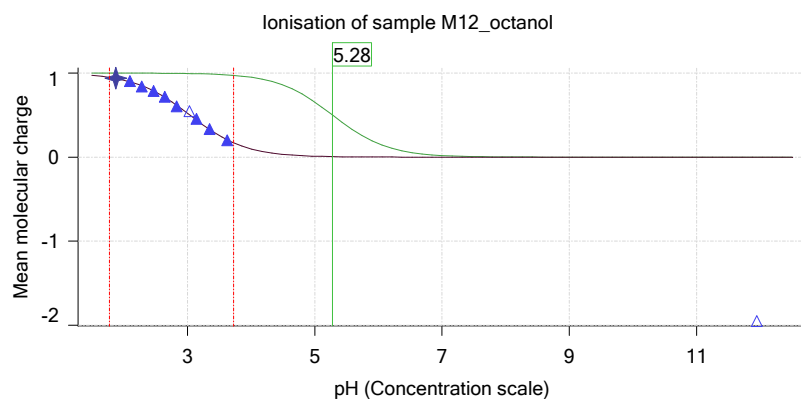
Titrants

0.50 M HCl 0.999058 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 0.50 M KOH 0.999845 3/3/2018 7:38:51 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M12_octanol concentration factor 1.664
 M12_octanol stoichiometry 1.000
 Chloride stoichiometry 1.000
 Base pKa 1 5.28
 logP (XH +) 1.02
 logP (neutral X) 3.89

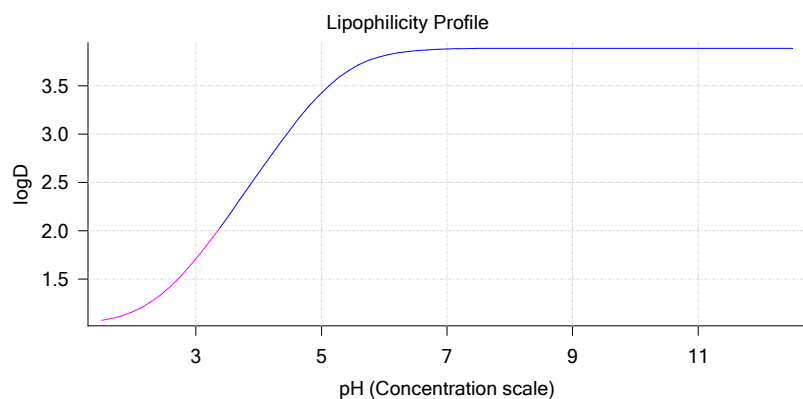
Sample graphs



Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**


Sample graphs (continued)



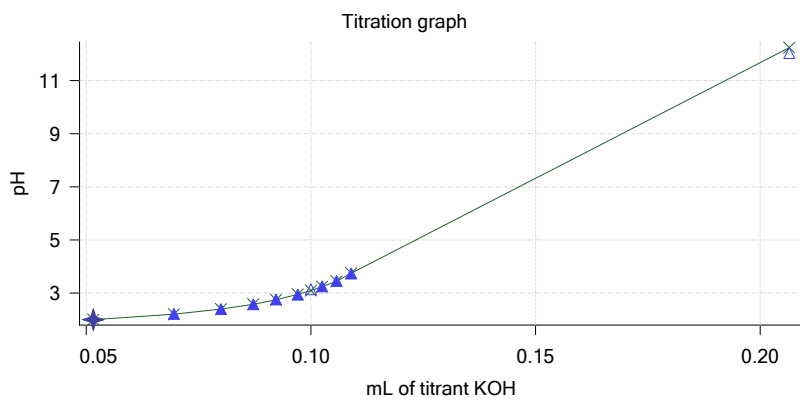
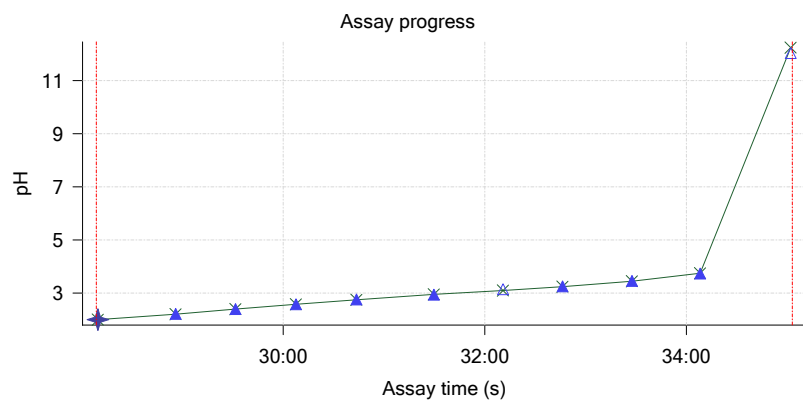
Sample logD and percent species

pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanolH	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.04	75.84 %	0.00 %	23.25 %	0.90 %	Stomach pH
1.200	1.05	75.44 %	0.01 %	23.13 %	1.43 %	
2.000	1.16	70.11 %	0.04 %	21.50 %	8.36 %	
3.000	1.71	39.94 %	0.21 %	12.25 %	47.60 %	
4.000	2.60	7.53 %	0.40 %	2.31 %	89.76 %	
5.000	3.43	0.83 %	0.43 %	0.25 %	98.49 %	
6.000	3.81	0.08 %	0.44 %	0.03 %	99.45 %	Blood pH
6.500	3.86	0.03 %	0.44 %	0.01 %	99.53 %	
7.000	3.88	0.01 %	0.44 %	0.00 %	99.55 %	
7.400	3.89	0.00 %	0.44 %	0.00 %	99.56 %	
8.000	3.89	0.00 %	0.44 %	0.00 %	99.56 %	
9.000	3.89	0.00 %	0.44 %	0.00 %	99.56 %	
10.000	3.89	0.00 %	0.44 %	0.00 %	99.56 %	
11.000	3.89	0.00 %	0.44 %	0.00 %	99.56 %	
12.000	3.89	0.00 %	0.44 %	0.00 %	99.56 %	

Carbonate and acidity

 Carbonate 0.134 mM
 Acidity error -2.741 mM

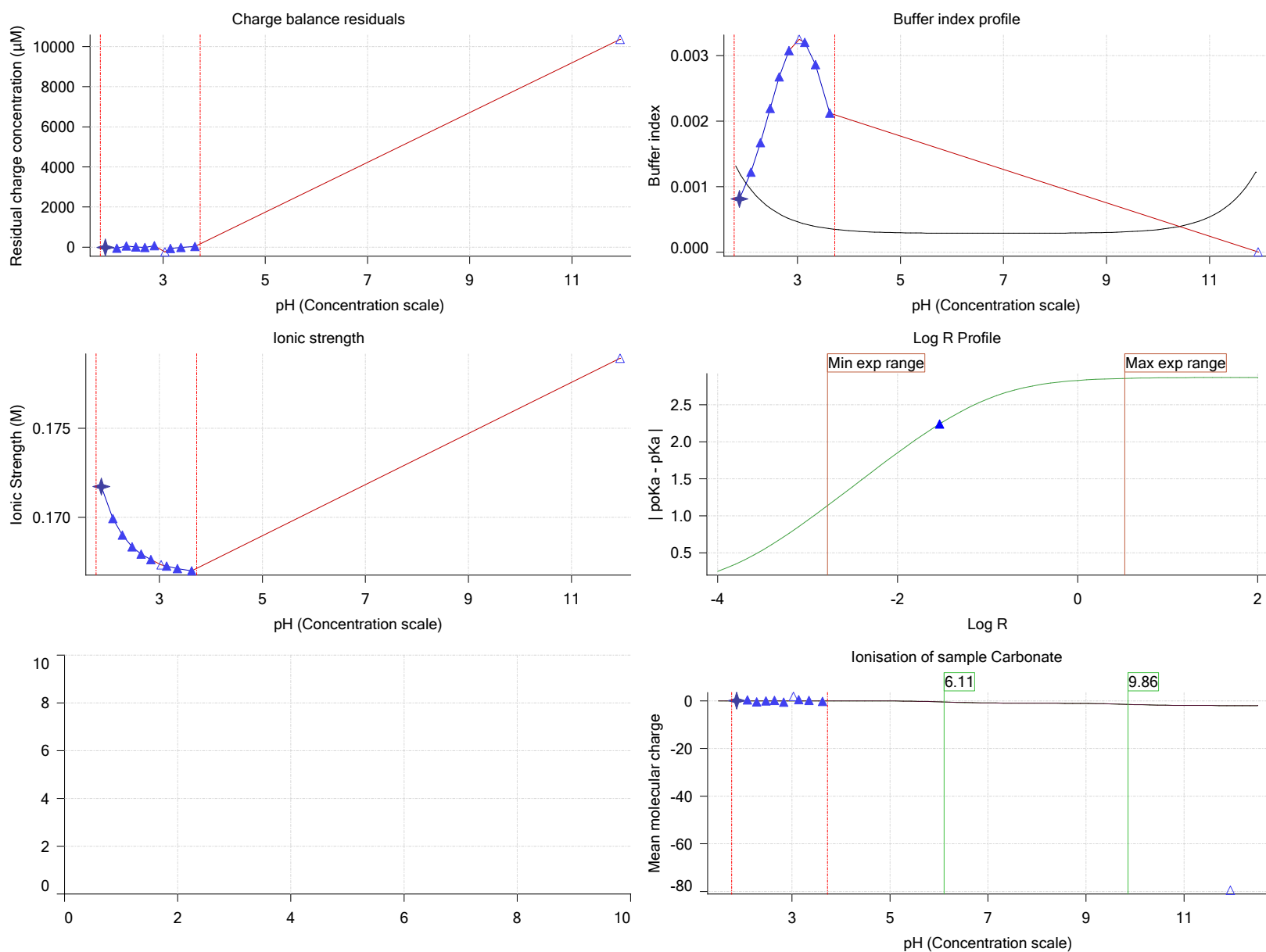
Other graphs



Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M12_octanol** Experiment start time: **3/3/2018 7:38:51 PM**
 Assay name: **pH-metric high logP** Analyst: **Pion**
 Assay ID: **18C-03015** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

pH-metric high logP Titration 3 of 3 18C-03015 Points 30 to 56





Overall results

RMSD 0.199
 Average ionic strength 0.181 M
 Average temperature 25.0°C
 Partition ratio 0.1256 : 1
 Analyte concentration range 2574.7 µM to 2650.8 µM
 Total points considered 20 of 27



Warnings and errors

Errors None
 Warnings Excessive acidity error present







Four-Plus parameters

 Alpha 0.111 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 S 0.9988 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 jH 1.0 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 jOH -0.8 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r

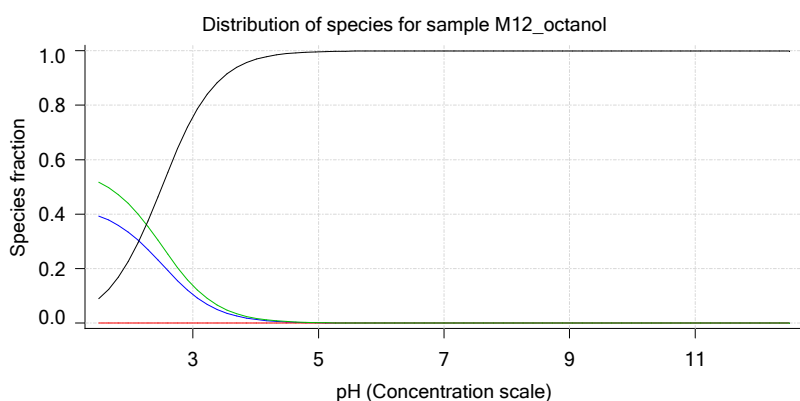
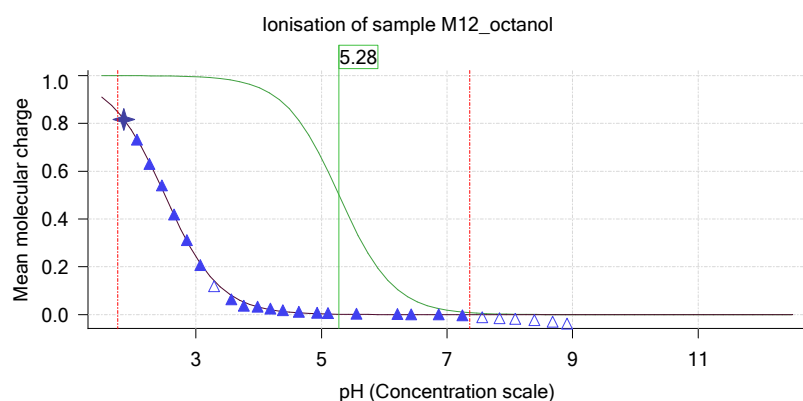
Titrants

 0.50 M HCl 0.999058 3/3/2018 7:38:51 PM C:\Sirius_T3\HCl18C02.t3r
 0.50 M KOH 0.999845 3/3/2018 7:38:51 PM C:\Sirius_T3\KOH18B27.t3r

Sample

 M12_octanol concentration factor 0.918
 M12_octanol stoichiometry 1.000
 Chloride stoichiometry 1.000
 Base pKa 1 5.28
 logP (XH +) 1.02
 logP (neutral X) 4.04

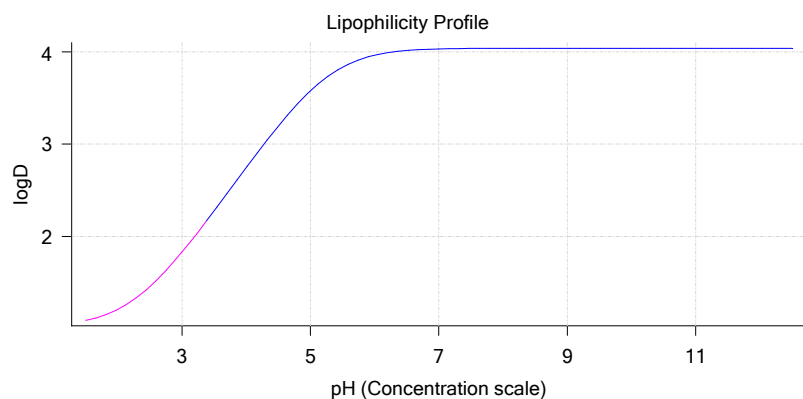
Sample graphs



Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
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 Instrument ID: **T312060**

Sample graphs (continued)



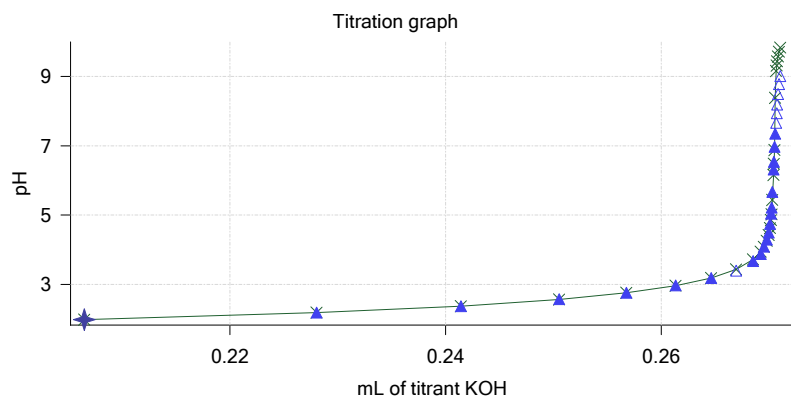
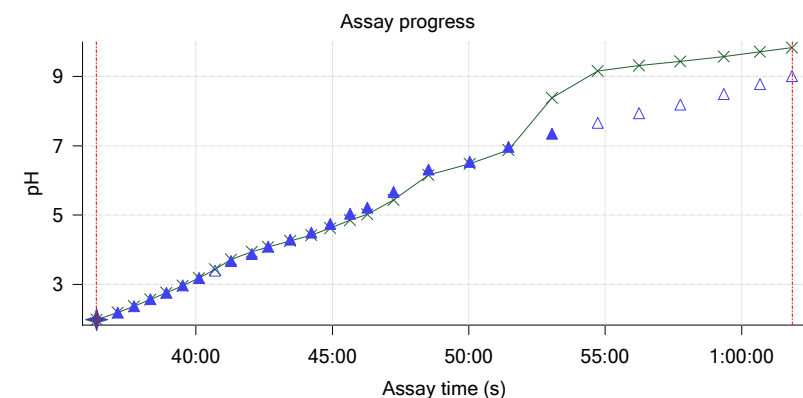
Sample logD and percent species

pH	M12_octanol logD	M12_octanol M12_octanolH	M12_octanol M12_octanolH	M12_octanol M12_octanolH*	M12_octanol M12_octanol*	Comment
1.000	1.04	41.89 %	0.00 %	55.08 %	3.02 %	Stomach pH
1.200	1.06	41.16 %	0.00 %	54.12 %	4.71 %	
2.000	1.21	32.92 %	0.02 %	43.29 %	23.77 %	
3.000	1.83	10.48 %	0.06 %	13.78 %	75.68 %	
4.000	2.75	1.34 %	0.07 %	1.76 %	96.83 %	
5.000	3.58	0.14 %	0.07 %	0.18 %	99.61 %	Blood pH
6.000	3.96	0.01 %	0.07 %	0.02 %	99.90 %	
6.500	4.01	0.00 %	0.07 %	0.01 %	99.92 %	
7.000	4.03	0.00 %	0.07 %	0.00 %	99.92 %	
7.400	4.04	0.00 %	0.07 %	0.00 %	99.93 %	
8.000	4.04	0.00 %	0.07 %	0.00 %	99.93 %	
9.000	4.04	0.00 %	0.07 %	0.00 %	99.93 %	
10.000	4.04	0.00 %	0.07 %	0.00 %	99.93 %	
11.000	4.04	0.00 %	0.07 %	0.00 %	99.93 %	
12.000	4.04	0.00 %	0.07 %	0.00 %	99.93 %	

Carbonate and acidity

Carbonate 0.057 mM
 Acidity error 8.572 mM

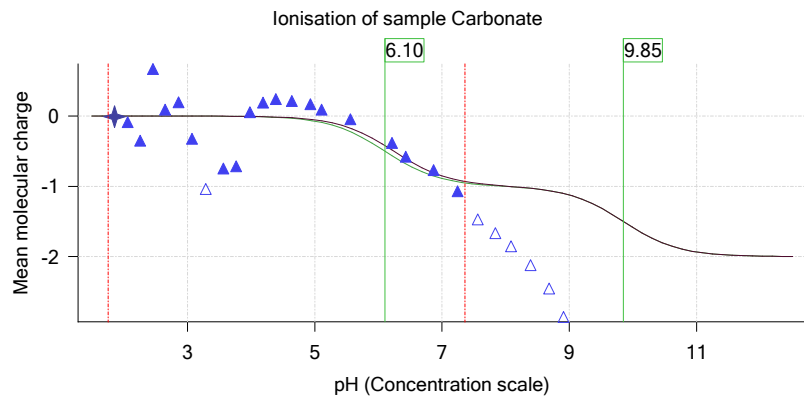
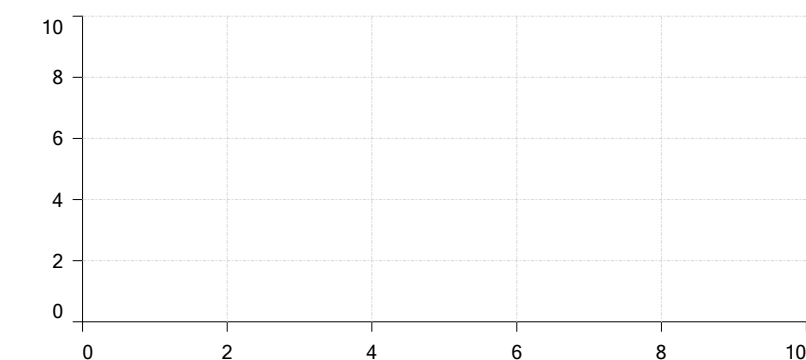
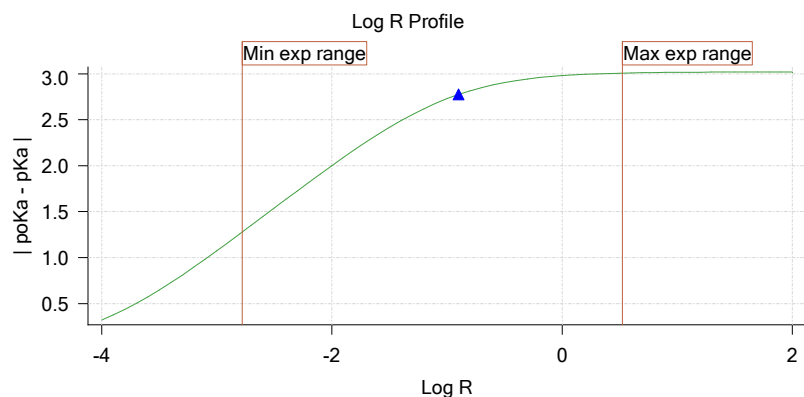
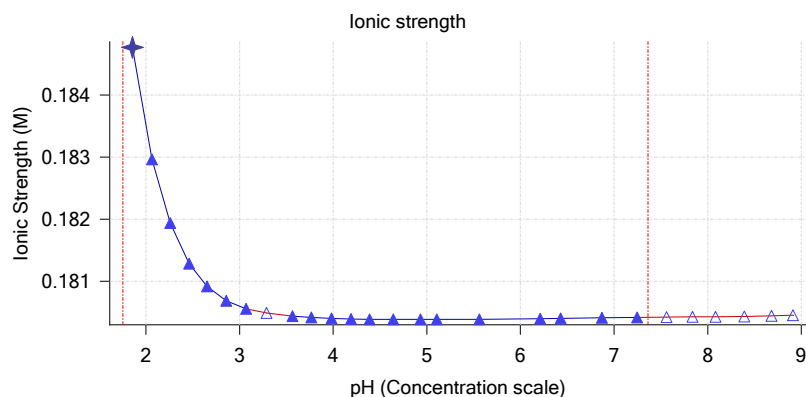
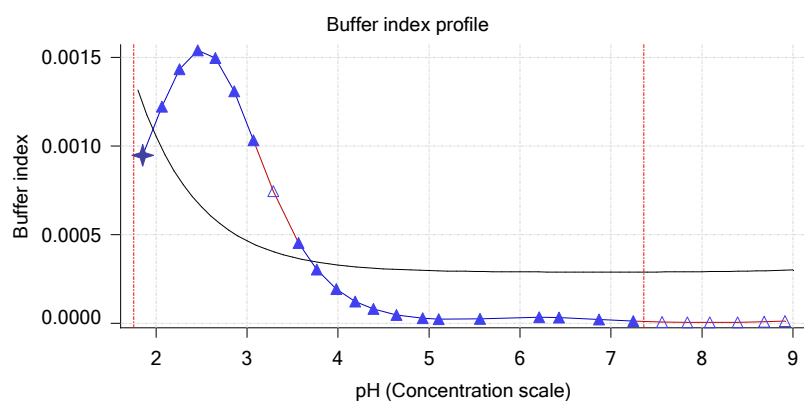
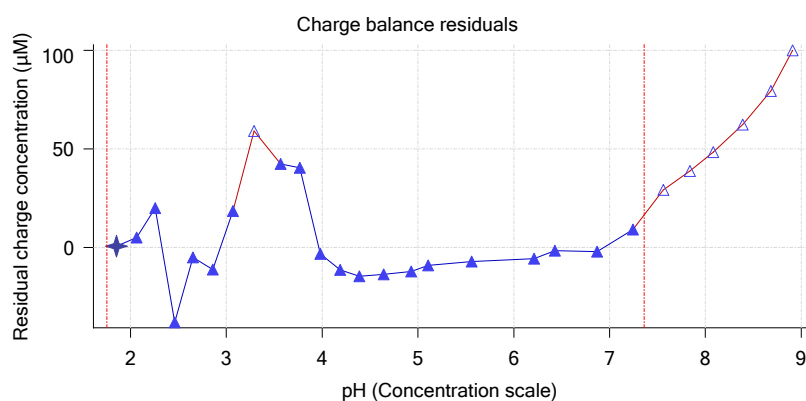
Other graphs



Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M12_octanol	2/28/2018 2:58:36 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001690 g	3/2/2018 5:10:33 PM	User entered value
Formula weight	292.16 g/mol	2/28/2018 2:58:36 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	255.70	2/28/2018 2:58:36 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/28/2018 2:58:36 PM	User entered value
Sample is a	Base	2/28/2018 2:58:36 PM	User entered value
pKa 1	5.28	2/28/2018 2:58:36 PM	User entered value
logp (XH +)	1.02	3/2/2018 3:44:28 PM	User entered value
logP (neutral X)	3.79	3/2/2018 3:44:35 PM	User entered value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
5:59.8	Initial pH = 4.05									
8:59.2	Data point 1	1.50000 mL	0.04798 mL	0.00233 mL	0.01999 mL	2.090	-0.00070	0.00914	0.00036	10.0 s
9:45.4	Data point 2	1.50000 mL	0.04798 mL	0.01717 mL	0.01999 mL	2.312	-0.00312	0.68871	0.00019	10.5 s
10:31.9	Data point 3	1.50000 mL	0.04798 mL	0.02629 mL	0.01999 mL	2.526	0.00243	0.06275	0.00048	10.5 s
11:18.4	Data point 4	1.50000 mL	0.04798 mL	0.03248 mL	0.01999 mL	2.730	-0.00626	0.82301	0.00034	10.0 s
12:04.3	Data point 5	1.50000 mL	0.04798 mL	0.03631 mL	0.01999 mL	2.938	-0.00734	0.94317	0.00037	10.5 s
12:40.3	Data point 6	1.50000 mL	0.04798 mL	0.03899 mL	0.01999 mL	3.110	-0.01187	0.90433	0.00062	10.0 s
13:31.5	Data point 7	1.50000 mL	0.04798 mL	0.04433 mL	0.01999 mL	3.640	-0.01726	0.73640	0.00099	11.5 s
14:23.9	Data point 8	1.50000 mL	0.04798 mL	0.04605 mL	0.01999 mL	3.809	-0.01938	0.96322	0.00098	15.0 s
15:04.4	Data point 9	1.50000 mL	0.04798 mL	0.04739 mL	0.01999 mL	4.005	-0.01944	0.95579	0.00098	12.0 s
15:41.8	Data point 10	1.50000 mL	0.04798 mL	0.04845 mL	0.01999 mL	4.191	-0.01847	0.88746	0.00097	13.5 s
16:20.8	Data point 11	1.50000 mL	0.04798 mL	0.04922 mL	0.01999 mL	4.372	-0.01878	0.94552	0.00095	23.5 s
17:14.9	Data point 12	1.50000 mL	0.04798 mL	0.05024 mL	0.01999 mL	4.829	-0.01888	0.96108	0.00095	30.0 s
18:15.5	Data point 13	1.50000 mL	0.04798 mL	0.05085 mL	0.01999 mL	5.982	-0.01949	0.93892	0.00099	52.5 s
19:49.0	Data point 14	1.50000 mL	0.04798 mL	0.05111 mL	0.01999 mL	6.938	-0.03568	0.99301	0.00177	Timed out at 59.5 s
21:24.6	Data point 15	1.50000 mL	0.04798 mL	0.05118 mL	0.01999 mL	7.503	-0.03856	0.98751	0.00192	Timed out at 59.5 s
23:00.2	Data point 16	1.50000 mL	0.04798 mL	0.05125 mL	0.01999 mL	7.986	-0.04249	0.99373	0.00210	Timed out at 59.5 s
24:41.0	Data point 17	1.50000 mL	0.04798 mL	0.05134 mL	0.01999 mL	8.384	-0.03068	0.99526	0.00152	Timed out at 59.5 s
26:21.7	Data point 18	1.50000 mL	0.04798 mL	0.05158 mL	0.01999 mL	9.153	-0.01970	0.96174	0.00099	49.0 s
28:09.7	Data point 19	1.50000 mL	0.10388 mL	0.05158 mL	0.05000 mL	1.995	-0.00675	0.60729	0.00043	10.0 s
28:55.9	Data point 20	1.50000 mL	0.10388 mL	0.06954 mL	0.05000 mL	2.211	-0.00301	0.08351	0.00051	10.0 s
29:31.6	Data point 21	1.50000 mL	0.10388 mL	0.08001 mL	0.05000 mL	2.394	0.00217	0.25971	0.00021	10.5 s
30:07.6	Data point 22	1.50000 mL	0.10388 mL	0.08718 mL	0.05000 mL	2.582	0.01006	0.35818	0.00083	10.5 s
30:43.7	Data point 23	1.50000 mL	0.10388 mL	0.09226 mL	0.05000 mL	2.754	-0.00412	0.68848	0.00025	10.0 s
31:29.7	Data point 24	1.50000 mL	0.10388 mL	0.09711 mL	0.05000 mL	2.942	-0.00701	0.24786	0.00069	10.5 s
32:10.9	Data point 25	1.50000 mL	0.10388 mL	0.10002 mL	0.05000 mL	3.142	-0.00388	0.12360	0.00054	10.0 s
32:46.3	Data point 26	1.50000 mL	0.10388 mL	0.10249 mL	0.05000 mL	3.250	-0.00583	0.78197	0.00033	10.5 s
33:27.5	Data point 27	1.50000 mL	0.10388 mL	0.10574 mL	0.05000 mL	3.456	-0.01149	0.59025	0.00074	10.0 s
34:08.3	Data point 28	1.50000 mL	0.10388 mL	0.10898 mL	0.05000 mL	3.732	0.00666	0.19651	0.00074	10.5 s
35:02.1	Data point 29	1.50000 mL	0.10388 mL	0.20652 mL	0.05000 mL	12.026	0.00788	0.91250	0.00041	10.5 s
36:22.1	Data point 30	1.50000 mL	0.22564 mL	0.20652 mL	0.25000 mL	1.977	-0.01444	0.92481	0.00074	10.0 s
37:08.5	Data point 31	1.50000 mL	0.22564 mL	0.22803 mL	0.25000 mL	2.180	-0.00826	0.64596	0.00051	10.0 s
37:44.3	Data point 32	1.50000 mL	0.22564 mL	0.24142 mL	0.25000 mL	2.372	-0.00705	0.53601	0.00048	10.0 s



Assay Events

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03015**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
38:19.9	Data point 33	1.50000 mL	0.22564 mL	0.25052 mL	0.25000 mL	2.571	-0.00201	0.05339	0.00043	10.0 s
38:55.5	Data point 34	1.50000 mL	0.22564 mL	0.25677 mL	0.25000 mL	2.761	-0.00400	0.13797	0.00053	10.0 s
39:31.1	Data point 35	1.50000 mL	0.22564 mL	0.26134 mL	0.25000 mL	2.967	-0.00538	0.70571	0.00032	10.0 s
40:06.6	Data point 36	1.50000 mL	0.22564 mL	0.26463 mL	0.25000 mL	3.179	-0.00342	0.11319	0.00050	10.0 s
40:42.1	Data point 37	1.50000 mL	0.22564 mL	0.26693 mL	0.25000 mL	3.396	-0.00748	0.56380	0.00049	10.0 s
41:17.6	Data point 38	1.50000 mL	0.22564 mL	0.26851 mL	0.25000 mL	3.672	-0.00209	0.04091	0.00051	10.0 s
42:03.3	Data point 39	1.50000 mL	0.22564 mL	0.26921 mL	0.25000 mL	3.873	-0.00392	0.08581	0.00066	10.0 s
42:38.7	Data point 40	1.50000 mL	0.22564 mL	0.26952 mL	0.25000 mL	4.087	-0.00077	0.00175	0.00091	18.0 s
43:27.2	Data point 41	1.50000 mL	0.22564 mL	0.26978 mL	0.25000 mL	4.294	-0.00113	0.00401	0.00088	10.5 s
44:13.6	Data point 42	1.50000 mL	0.22564 mL	0.26994 mL	0.25000 mL	4.494	-0.00826	0.23363	0.00084	11.0 s
44:55.1	Data point 43	1.50000 mL	0.22564 mL	0.27009 mL	0.25000 mL	4.746	-0.01490	0.56284	0.00098	18.5 s
45:39.0	Data point 44	1.50000 mL	0.22564 mL	0.27018 mL	0.25000 mL	5.035	-0.01117	0.33968	0.00095	12.5 s
46:16.9	Data point 45	1.50000 mL	0.22564 mL	0.27023 mL	0.25000 mL	5.210	-0.01900	0.90187	0.00099	27.5 s
47:14.9	Data point 46	1.50000 mL	0.22564 mL	0.27030 mL	0.25000 mL	5.664	-0.01760	0.93799	0.00090	46.0 s
48:31.5	Data point 47	1.50000 mL	0.22564 mL	0.27039 mL	0.25000 mL	6.314	-0.03485	0.93285	0.00178	Timed out at 59.5 s
50:02.1	Data point 48	1.50000 mL	0.22564 mL	0.27044 mL	0.25000 mL	6.532	-0.03321	0.95029	0.00168	Timed out at 59.5 s
51:27.4	Data point 49	1.50000 mL	0.22564 mL	0.27048 mL	0.25000 mL	6.971	-0.05095	0.98242	0.00254	Timed out at 59.5 s
53:03.0	Data point 50	1.50000 mL	0.22564 mL	0.27055 mL	0.25000 mL	7.347	-0.06715	0.99206	0.00333	Timed out at 59.5 s
54:43.9	Data point 51	1.50000 mL	0.22564 mL	0.27065 mL	0.25000 mL	7.663	-0.06618	0.98872	0.00329	Timed out at 59.5 s
56:14.4	Data point 52	1.50000 mL	0.22564 mL	0.27070 mL	0.25000 mL	7.938	-0.05473	0.99204	0.00271	Timed out at 59.5 s
57:44.9	Data point 53	1.50000 mL	0.22564 mL	0.27074 mL	0.25000 mL	8.184	-0.04284	0.94491	0.00218	Timed out at 59.5 s
59:20.6	Data point 54	1.50000 mL	0.22564 mL	0.27081 mL	0.25000 mL	8.490	-0.00848	0.37648	0.00068	38.5 s
1:00:40.1	Data point 55	1.50000 mL	0.22564 mL	0.27091 mL	0.25000 mL	8.782	-0.00488	0.07901	0.00086	29.5 s
1:01:50.4	Data point 56	1.50000 mL	0.22564 mL	0.27103 mL	0.25000 mL	9.009	-0.01631	0.80065	0.00090	14.5 s
1:02:13.9	Assay volumes	1.50000 mL	0.22564 mL	0.27103 mL	0.25000 mL					

Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.030 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.111	3/3/2018 7:38:51 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus S	0.9988	3/3/2018 7:38:51 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jH	1.0	3/3/2018 7:38:51 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jOH	-0.8	3/3/2018 7:38:51 PM	C:\Sirius_T3\HCl18C02.t3r
Base concentration factor	1.000	3/3/2018 7:38:51 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.999	3/3/2018 7:38:51 PM	C:\Sirius_T3\HCl18C02.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M12_octanol** Experiment start time: **3/3/2018 7:38:51 PM**
 Assay name: **pH-metric high logP** Analyst: **Pion**
 Assay ID: **18C-03015** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+5.90 mV		3/3/2018 7:39:19 PM
Filling solution	3M KCl	KCL097	3/2/2018 9:43:24 AM
Liquids			
Wash 1	50% IPA:50% Water		3/2/2018 9:45:12 AM
Wash 2	0.5% Triton X-100 in H2O		3/2/2018 9:45:15 AM
Buffer position 1	pH7 Wash		3/2/2018 9:45:18 AM
Buffer position 2	pH 7		3/2/2018 9:45:21 AM
Storage position			3/2/2018 9:44:44 AM
Wash water	6.6e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	8.9e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	120:41:49		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name:	M12_octanol	Experiment start time:	3/3/2018 7:38:51 PM
Assay name:	pH-metric high logP	Analyst:	Pion
Assay ID:	18C-03015	Instrument ID:	T312060
Filename:	C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r		

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:37] Air gap created for Water (0.15 M KCl)
 [2:37] Air gap created for Acid (0.5 M HCl)
 [2:38] Air gap created for Base (0.5 M KOH)
 [2:38] Air gap released for Water (0.15 M KCl)
 [2:42] Titrator arm moved over Titration position
 [2:42] Titration 1 of 3
 [2:42] Adding initial titrants
 [2:42] Automatically add 1.50000 mL of water
 [3:07] Dispensed 1.500000 mL of Water (0.15 M KCl)
 [3:11] Titrator arm moved over Drain
 [5:53] Titrator arm moved to Titration position
 [5:53] Argon flow rate set to 100
 [5:53] Stirrer speed set to 10
 [5:58] Automatically add 0.02000 mL of Octanol
 [5:58] Dispensed 0.019991 mL of Octanol
 [6:00] Initial pH = 4.05
 [6:00] Iterative adjust 4.05 -> 2.00
 [6:00] pH 4.05 -> 2.00
 [6:01] Air gap released for Acid (0.5 M HCl)
 [6:02] Dispensed 0.047977 mL of Acid (0.5 M HCl)
 [6:07] Holding pH 2.00
 [8:07] Stirrer speed set to 0
 [8:07] Stirrer speed set to 50
 [8:07] Iterative adjust 1.98 -> 2.00
 [8:07] pH 1.98 -> 2.00
 [8:08] Air gap released for Base (0.5 M KOH)
 [8:09] Dispensed 0.002328 mL of Base (0.5 M KOH)
 [8:59] Stirrer speed set to 0
 [9:09] Datapoint id 1 collected
 [9:09] Stirrer speed set to 50
 [9:14] pH 2.10 -> 2.30
 [9:14] Using cautious pH adjust
 [9:14] Dispensed 0.006232 mL of Base (0.5 M KOH)
 [9:19] Stepping pH = 2.16
 [9:20] Dispensed 0.006726 mL of Base (0.5 M KOH)
 [9:25] Stepping pH = 2.26
 [9:25] Dispensed 0.001881 mL of Base (0.5 M KOH)
 [9:30] Stepping pH = 2.31
 [9:45] Stirrer speed set to 0
 [9:56] Datapoint id 2 collected
 [9:56] Charge balance equation is out by -18.9%
 [9:56] Stirrer speed set to 50

Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Experiment Log (continued)

[10:01] pH 2.32 -> 2.52
 [10:01] Using cautious pH adjust
 [10:01] Dispensed 0.003810 mL of Base (0.5 M KOH)
 [10:06] Stepping pH = 2.39
 [10:06] Dispensed 0.004186 mL of Base (0.5 M KOH)
 [10:11] Stepping pH = 2.49
 [10:12] Dispensed 0.001129 mL of Base (0.5 M KOH)
 [10:17] Stepping pH = 2.53
 [10:32] Stirrer speed set to 0
 [10:42] Datapoint id 3 collected
 [10:42] Charge balance equation is out by -19.8%
 [10:42] Stirrer speed set to 50
 [10:47] pH 2.54 -> 2.74
 [10:47] Using cautious pH adjust
 [10:48] Dispensed 0.002469 mL of Base (0.5 M KOH)
 [10:53] Stepping pH = 2.60
 [10:53] Dispensed 0.002893 mL of Base (0.5 M KOH)
 [10:58] Stepping pH = 2.70
 [10:58] Dispensed 0.000823 mL of Base (0.5 M KOH)
 [11:03] Stepping pH = 2.73
 [11:18] Stirrer speed set to 0
 [11:28] Datapoint id 4 collected
 [11:28] Charge balance equation is out by -25.7%
 [11:28] Stirrer speed set to 50
 [11:33] pH 2.74 -> 2.94
 [11:33] Using cautious pH adjust
 [11:34] Dispensed 0.001740 mL of Base (0.5 M KOH)
 [11:39] Stepping pH = 2.82
 [11:39] Dispensed 0.001599 mL of Base (0.5 M KOH)
 [11:44] Stepping pH = 2.90
 [11:44] Dispensed 0.000494 mL of Base (0.5 M KOH)
 [11:49] Stepping pH = 2.94
 [12:04] Stirrer speed set to 0
 [12:15] Datapoint id 5 collected
 [12:15] Charge balance equation is out by -9.6%
 [12:15] Stirrer speed set to 50
 [12:20] pH 2.94 -> 3.14
 [12:20] Using charge balance adjust
 [12:20] Dispensed 0.002681 mL of Base (0.5 M KOH)
 [12:40] Stirrer speed set to 0
 [12:50] Datapoint id 6 collected
 [12:50] Charge balance equation is out by -17.5%
 [12:50] Stirrer speed set to 50
 [12:55] pH 3.11 -> 3.31
 [12:55] Using cautious pH adjust
 [12:55] Dispensed 0.001152 mL of Base (0.5 M KOH)
 [13:01] Stepping pH = 3.19
 [13:01] Dispensed 0.001129 mL of Base (0.5 M KOH)
 [13:06] Stepping pH = 3.27
 [13:06] Dispensed 0.000447 mL of Base (0.5 M KOH)
 [13:11] Stepping pH = 3.27
 [13:11] Dispensed 0.002611 mL of Base (0.5 M KOH)
 [13:16] Stepping pH = 3.68
 [13:31] Stirrer speed set to 0
 [13:43] Datapoint id 7 collected
 [13:43] Charge balance equation is out by -131.1%
 [13:43] Stirrer speed set to 50
 [13:48] pH 3.65 -> 3.85
 [13:48] Using cautious pH adjust

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03015**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[13:48] Dispensed 0.000800 mL of Base (0.5 M KOH)
[13:53] Stepping pH = 3.73
[13:53] Dispensed 0.000682 mL of Base (0.5 M KOH)
[13:58] Stepping pH = 3.83
[13:58] Dispensed 0.000094 mL of Base (0.5 M KOH)
[14:03] Stepping pH = 3.83
[14:04] Dispensed 0.000141 mL of Base (0.5 M KOH)
[14:09] Stepping pH = 3.85
[14:24] Stirrer speed set to 0
[14:39] Datapoint id 8 collected
[14:39] Charge balance equation is out by -7.4%
[14:39] Stirrer speed set to 50
[14:44] pH 3.82 -> 4.02
[14:44] Using charge balance adjust
[14:44] Dispensed 0.001341 mL of Base (0.5 M KOH)
[15:04] Stirrer speed set to 0
[15:16] Datapoint id 9 collected
[15:16] Charge balance equation is out by -8.5%
[15:16] Stirrer speed set to 50
[15:21] pH 4.01 -> 4.21
[15:21] Using charge balance adjust
[15:21] Dispensed 0.001058 mL of Base (0.5 M KOH)
[15:42] Stirrer speed set to 0
[15:55] Datapoint id 10 collected
[15:55] Charge balance equation is out by -11.1%
[15:55] Stirrer speed set to 50
[16:00] pH 4.21 -> 4.41
[16:00] Using charge balance adjust
[16:00] Dispensed 0.000776 mL of Base (0.5 M KOH)
[16:21] Stirrer speed set to 0
[16:44] Datapoint id 11 collected
[16:44] Charge balance equation is out by -19.6%
[16:44] Stirrer speed set to 50
[16:49] pH 4.41 -> 4.61
[16:49] Using cautious pH adjust
[16:49] Dispensed 0.000282 mL of Base (0.5 M KOH)
[16:54] Stepping pH = 4.43
[16:55] Dispensed 0.000729 mL of Base (0.5 M KOH)
[17:00] Stepping pH = 4.88
[17:15] Stirrer speed set to 0
[17:45] Datapoint id 12 collected
[17:45] Charge balance equation is out by -84.8%
[17:45] Stirrer speed set to 50
[17:50] pH 4.90 -> 5.10
[17:50] Using cautious pH adjust
[17:50] Dispensed 0.000094 mL of Base (0.5 M KOH)
[17:55] Stepping pH = 4.89
[17:55] Dispensed 0.000517 mL of Base (0.5 M KOH)
[18:00] Stepping pH = 5.56
[18:15] Stirrer speed set to 0
[19:08] Datapoint id 13 collected
[19:08] Charge balance equation is out by -203.9%
[19:08] Stirrer speed set to 50
[19:13] pH 6.15 -> 6.35
[19:13] Using cautious pH adjust
[19:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[19:18] Stepping pH = 6.19
[19:18] Dispensed 0.000047 mL of Base (0.5 M KOH)
[19:23] Stepping pH = 6.22

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03015**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[19:23] Dispensed 0.000094 mL of Base (0.5 M KOH)
[19:29] Stepping pH = 6.26
[19:29] Dispensed 0.000094 mL of Base (0.5 M KOH)
[19:34] Stepping pH = 6.43
[19:49] Stirrer speed set to 0
[20:49] Datapoint id 14 collected
[20:49] Charge balance equation is out by -426.3%
[20:49] Stirrer speed set to 50
[20:54] pH 7.06 -> 7.26
[20:54] Using cautious pH adjust
[20:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[20:59] Stepping pH = 7.13
[20:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[21:04] Stepping pH = 7.20
[21:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[21:09] Stepping pH = 7.31
[21:24] Stirrer speed set to 0
[22:24] Datapoint id 15 collected
[22:24] Charge balance equation is out by -279.1%
[22:24] Stirrer speed set to 50
[22:29] pH 7.62 -> 7.82
[22:29] Using cautious pH adjust
[22:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[22:35] Stepping pH = 7.71
[22:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[22:40] Stepping pH = 7.77
[22:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[22:45] Stepping pH = 7.83
[23:00] Stirrer speed set to 0
[24:00] Datapoint id 16 collected
[24:00] Charge balance equation is out by -785.0%
[24:00] Stirrer speed set to 50
[24:05] pH 8.16 -> 8.36
[24:05] Using cautious pH adjust
[24:05] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:10] Stepping pH = 8.25
[24:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:15] Stepping pH = 8.30
[24:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:21] Stepping pH = 8.32
[24:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:26] Stepping pH = 8.35
[24:41] Stirrer speed set to 0
[25:41] Datapoint id 17 collected
[25:41] Charge balance equation is out by -917.7%
[25:41] Stirrer speed set to 50
[25:46] pH 8.43 -> 8.63
[25:46] Using cautious pH adjust
[25:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[25:51] Stepping pH = 8.44
[25:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[25:56] Stepping pH = 8.44
[25:56] Dispensed 0.000047 mL of Base (0.5 M KOH)
[26:01] Stepping pH = 8.46
[26:01] Dispensed 0.000141 mL of Base (0.5 M KOH)
[26:06] Stepping pH = 8.83
[26:22] Stirrer speed set to 0
[27:11] Datapoint id 18 collected
[27:11] Charge balance equation is out by -1,849.5%

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03015**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[27:11] Titration 2 of 3
[27:11] Adding initial titrants
[27:11] Automatically add 0.03000 mL of Octanol
[27:11] Dispensed 0.030009 mL of Octanol
[27:11] Stirrer speed set to 10
[27:13] Stirrer speed set to 55
[27:13] Iterative adjust 9.17 -> 2.00
[27:13] pH 9.17 -> 2.00
[27:14] Dispensed 0.053763 mL of Acid (0.5 M HCl)
[27:19] pH 2.02 -> 2.00
[27:19] Dispensed 0.002140 mL of Acid (0.5 M HCl)
[28:09] Stirrer speed set to 0
[28:19] Datapoint id 19 collected
[28:19] Stirrer speed set to 55
[28:25] pH 2.01 -> 2.21
[28:25] Using cautious pH adjust
[28:25] Dispensed 0.008208 mL of Base (0.5 M KOH)
[28:30] Stepping pH = 2.09
[28:30] Dispensed 0.007785 mL of Base (0.5 M KOH)
[28:35] Stepping pH = 2.18
[28:36] Dispensed 0.001976 mL of Base (0.5 M KOH)
[28:41] Stepping pH = 2.21
[28:56] Stirrer speed set to 0
[29:06] Datapoint id 20 collected
[29:06] Charge balance equation is out by -9.5%
[29:06] Stirrer speed set to 55
[29:11] pH 2.22 -> 2.42
[29:11] Using charge balance adjust
[29:11] Dispensed 0.010466 mL of Base (0.5 M KOH)
[29:31] Stirrer speed set to 0
[29:42] Datapoint id 21 collected
[29:42] Charge balance equation is out by -10.6%
[29:42] Stirrer speed set to 55
[29:47] pH 2.40 -> 2.60
[29:47] Using charge balance adjust
[29:47] Dispensed 0.007173 mL of Base (0.5 M KOH)
[30:07] Stirrer speed set to 0
[30:18] Datapoint id 22 collected
[30:18] Charge balance equation is out by -9.0%
[30:18] Stirrer speed set to 55
[30:23] pH 2.59 -> 2.79
[30:23] Using charge balance adjust
[30:23] Dispensed 0.005080 mL of Base (0.5 M KOH)
[30:43] Stirrer speed set to 0
[30:53] Datapoint id 23 collected
[30:53] Charge balance equation is out by -17.4%
[30:53] Stirrer speed set to 55
[30:59] pH 2.76 -> 2.96
[30:59] Using cautious pH adjust
[30:59] Dispensed 0.001952 mL of Base (0.5 M KOH)
[31:04] Stepping pH = 2.83
[31:04] Dispensed 0.002070 mL of Base (0.5 M KOH)
[31:09] Stepping pH = 2.91
[31:09] Dispensed 0.000823 mL of Base (0.5 M KOH)
[31:14] Stepping pH = 2.95
[31:29] Stirrer speed set to 0
[31:40] Datapoint id 24 collected
[31:40] Charge balance equation is out by -23.5%
[31:40] Stirrer speed set to 55

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03015**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[31:45] pH 2.95 -> 3.15
[31:45] Using cautious pH adjust
[31:45] Dispensed 0.001552 mL of Base (0.5 M KOH)
[31:50] Stepping pH = 3.03
[31:50] Dispensed 0.001364 mL of Base (0.5 M KOH)
[31:56] Stepping pH = 3.15
[32:11] Stirrer speed set to 0
[32:21] Datapoint id 25 collected
[32:21] Charge balance equation is out by 5.6%
[32:21] Stirrer speed set to 55
[32:26] pH 3.15 -> 3.35
[32:26] Using charge balance adjust
[32:26] Dispensed 0.002469 mL of Base (0.5 M KOH)
[32:46] Stirrer speed set to 0
[32:57] Datapoint id 26 collected
[32:57] Charge balance equation is out by -50.0%
[32:57] Stirrer speed set to 55
[33:02] pH 3.25 -> 3.45
[33:02] Using cautious pH adjust
[33:02] Dispensed 0.001105 mL of Base (0.5 M KOH)
[33:07] Stepping pH = 3.29
[33:07] Dispensed 0.002140 mL of Base (0.5 M KOH)
[33:12] Stepping pH = 3.45
[33:27] Stirrer speed set to 0
[33:37] Datapoint id 27 collected
[33:37] Charge balance equation is out by -46.4%
[33:37] Stirrer speed set to 55
[33:42] pH 3.46 -> 3.66
[33:42] Using cautious pH adjust
[33:43] Dispensed 0.000870 mL of Base (0.5 M KOH)
[33:48] Stepping pH = 3.48
[33:48] Dispensed 0.002375 mL of Base (0.5 M KOH)
[33:53] Stepping pH = 3.75
[34:08] Stirrer speed set to 0
[34:19] Datapoint id 28 collected
[34:19] Charge balance equation is out by -87.2%
[34:19] Stirrer speed set to 55
[34:24] pH 3.74 -> 3.94
[34:24] Using cautious pH adjust
[34:24] Dispensed 0.000588 mL of Base (0.5 M KOH)
[34:29] Stepping pH = 3.73
[34:29] Dispensed 0.003057 mL of Base (0.5 M KOH)
[34:34] Stepping pH = 3.73
[34:35] Dispensed 0.015522 mL of Base (0.5 M KOH)
[34:40] Stepping pH = 3.73
[34:42] Dispensed 0.078363 mL of Base (0.5 M KOH)
[34:47] Stepping pH = 12.02
[35:02] Stirrer speed set to 0
[35:12] Datapoint id 29 collected
[35:12] Charge balance equation is out by -8,214.2%
[35:12] Titration 3 of 3
[35:12] Adding initial titrants
[35:12] Automatically add 0.20000 mL of Octanol
[35:17] Dispensed 0.200000 mL of Octanol
[35:17] Stirrer speed set to 10
[35:18] Stirrer speed set to 60
[35:18] Iterative adjust 12.03 -> 2.00
[35:18] pH 12.03 -> 2.00
[35:21] Dispensed 0.100000 mL of Acid (0.5 M HCl)

Sample name: **M12_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-03015**
 Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
 Analyst: **Pion**
 Instrument ID: **T312060**

Experiment Log (continued)

[35:26] pH 2.19 -> 2.00
 [35:26] Dispensed 0.018650 mL of Acid (0.5 M HCl)
 [35:31] pH 2.03 -> 2.00
 [35:32] Dispensed 0.003104 mL of Acid (0.5 M HCl)
 [36:22] Stirrer speed set to 0
 [36:32] Datapoint id 30 collected
 [36:32] Stirrer speed set to 60
 [36:37] pH 1.98 -> 2.18
 [36:37] Using cautious pH adjust
 [36:37] Dispensed 0.010348 mL of Base (0.5 M KOH)
 [36:42] Stepping pH = 2.07
 [36:43] Dispensed 0.008420 mL of Base (0.5 M KOH)
 [36:48] Stepping pH = 2.15
 [36:48] Dispensed 0.002752 mL of Base (0.5 M KOH)
 [36:53] Stepping pH = 2.18
 [37:08] Stirrer speed set to 0
 [37:18] Datapoint id 31 collected
 [37:18] Charge balance equation is out by -4.0%
 [37:18] Stirrer speed set to 60
 [37:23] pH 2.18 -> 2.38
 [37:23] Using charge balance adjust
 [37:24] Dispensed 0.013382 mL of Base (0.5 M KOH)
 [37:44] Stirrer speed set to 0
 [37:54] Datapoint id 32 collected
 [37:54] Charge balance equation is out by -6.2%
 [37:54] Stirrer speed set to 60
 [37:59] pH 2.38 -> 2.58
 [37:59] Using charge balance adjust
 [38:00] Dispensed 0.009102 mL of Base (0.5 M KOH)
 [38:20] Stirrer speed set to 0
 [38:30] Datapoint id 33 collected
 [38:30] Charge balance equation is out by -2.7%
 [38:30] Stirrer speed set to 60
 [38:35] pH 2.58 -> 2.78
 [38:35] Using charge balance adjust
 [38:35] Dispensed 0.006256 mL of Base (0.5 M KOH)
 [38:55] Stirrer speed set to 0
 [39:05] Datapoint id 34 collected
 [39:05] Charge balance equation is out by -9.2%
 [39:05] Stirrer speed set to 60
 [39:10] pH 2.77 -> 2.97
 [39:10] Using charge balance adjust
 [39:11] Dispensed 0.004563 mL of Base (0.5 M KOH)
 [39:31] Stirrer speed set to 0
 [39:41] Datapoint id 35 collected
 [39:41] Charge balance equation is out by -0.9%
 [39:41] Stirrer speed set to 60
 [39:46] pH 2.97 -> 3.17
 [39:46] Using charge balance adjust
 [39:46] Dispensed 0.003293 mL of Base (0.5 M KOH)
 [40:06] Stirrer speed set to 0
 [40:16] Datapoint id 36 collected
 [40:16] Charge balance equation is out by 3.4%
 [40:16] Stirrer speed set to 60
 [40:22] pH 3.18 -> 3.38
 [40:22] Using charge balance adjust
 [40:22] Dispensed 0.002305 mL of Base (0.5 M KOH)
 [40:42] Stirrer speed set to 0
 [40:52] Datapoint id 37 collected

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03015**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[40:52] Charge balance equation is out by 6.0%
[40:52] Stirrer speed set to 60
[40:57] pH 3.40 -> 3.60
[40:57] Using charge balance adjust
[40:57] Dispensed 0.001576 mL of Base (0.5 M KOH)
[41:17] Stirrer speed set to 0
[41:27] Datapoint id 38 collected
[41:27] Charge balance equation is out by 34.7%
[41:27] Stirrer speed set to 60
[41:32] pH 3.68 -> 3.88
[41:33] Using cautious pH adjust
[41:33] Dispensed 0.000447 mL of Base (0.5 M KOH)
[41:38] Stepping pH = 3.80
[41:38] Dispensed 0.000212 mL of Base (0.5 M KOH)
[41:43] Stepping pH = 3.87
[41:43] Dispensed 0.000047 mL of Base (0.5 M KOH)
[41:48] Stepping pH = 3.88
[42:03] Stirrer speed set to 0
[42:13] Datapoint id 39 collected
[42:13] Charge balance equation is out by 21.2%
[42:13] Stirrer speed set to 60
[42:18] pH 3.88 -> 4.08
[42:18] Using cautious pH adjust
[42:18] Dispensed 0.000306 mL of Base (0.5 M KOH)
[42:23] Stepping pH = 4.09
[42:38] Stirrer speed set to 0
[42:57] Datapoint id 40 collected
[42:57] Charge balance equation is out by 50.0%
[42:57] Stirrer speed set to 60
[43:02] pH 4.10 -> 4.30
[43:02] Using cautious pH adjust
[43:02] Dispensed 0.000188 mL of Base (0.5 M KOH)
[43:07] Stepping pH = 4.24
[43:07] Dispensed 0.000071 mL of Base (0.5 M KOH)
[43:12] Stepping pH = 4.29
[43:27] Stirrer speed set to 0
[43:38] Datapoint id 41 collected
[43:38] Charge balance equation is out by 32.9%
[43:38] Stirrer speed set to 60
[43:43] pH 4.32 -> 4.52
[43:43] Using cautious pH adjust
[43:43] Dispensed 0.000118 mL of Base (0.5 M KOH)
[43:48] Stepping pH = 4.48
[43:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[43:53] Stepping pH = 4.50
[43:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[43:58] Stepping pH = 4.51
[44:13] Stirrer speed set to 0
[44:24] Datapoint id 42 collected
[44:24] Charge balance equation is out by 33.2%
[44:24] Stirrer speed set to 60
[44:30] pH 4.50 -> 4.70
[44:30] Using cautious pH adjust
[44:30] Dispensed 0.000071 mL of Base (0.5 M KOH)
[44:35] Stepping pH = 4.58
[44:35] Dispensed 0.000071 mL of Base (0.5 M KOH)
[44:40] Stepping pH = 4.76
[44:55] Stirrer speed set to 0
[45:13] Datapoint id 43 collected

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03015**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[45:13] Charge balance equation is out by 6.7%
[45:13] Stirrer speed set to 60
[45:19] pH 4.82 -> 5.02
[45:19] Using charge balance adjust
[45:19] Dispensed 0.000094 mL of Base (0.5 M KOH)
[45:39] Stirrer speed set to 0
[45:51] Datapoint id 44 collected
[45:51] Charge balance equation is out by 9.7%
[45:51] Stirrer speed set to 60
[45:56] pH 5.11 -> 5.31
[45:56] Using charge balance adjust
[45:56] Dispensed 0.000047 mL of Base (0.5 M KOH)
[46:17] Stirrer speed set to 0
[46:44] Datapoint id 45 collected
[46:44] Charge balance equation is out by -48.8%
[46:44] Stirrer speed set to 60
[46:49] pH 5.25 -> 5.45
[46:49] Using cautious pH adjust
[46:49] Dispensed 0.000024 mL of Base (0.5 M KOH)
[46:54] Stepping pH = 5.29
[46:55] Dispensed 0.000047 mL of Base (0.5 M KOH)
[47:00] Stepping pH = 5.71
[47:15] Stirrer speed set to 0
[48:01] Datapoint id 46 collected
[48:01] Charge balance equation is out by -35.1%
[48:01] Stirrer speed set to 60
[48:06] pH 5.76 -> 5.96
[48:06] Using cautious pH adjust
[48:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[48:11] Stepping pH = 5.77
[48:11] Dispensed 0.000071 mL of Base (0.5 M KOH)
[48:16] Stepping pH = 6.49
[48:31] Stirrer speed set to 0
[49:31] Datapoint id 47 collected
[49:31] Charge balance equation is out by -96.3%
[49:31] Stirrer speed set to 60
[49:36] pH 6.31 -> 6.51
[49:36] Using cautious pH adjust
[49:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:42] Stepping pH = 6.43
[49:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:47] Stepping pH = 6.61
[50:02] Stirrer speed set to 0
[51:02] Datapoint id 48 collected
[51:02] Charge balance equation is out by 8.4%
[51:02] Stirrer speed set to 60
[51:07] pH 6.70 -> 6.90
[51:07] Using charge balance adjust
[51:07] Dispensed 0.000047 mL of Base (0.5 M KOH)
[51:27] Stirrer speed set to 0
[52:27] Datapoint id 49 collected
[52:27] Charge balance equation is out by 34.8%
[52:27] Stirrer speed set to 60
[52:32] pH 7.04 -> 7.24
[52:32] Using cautious pH adjust
[52:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[52:37] Stepping pH = 7.10
[52:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[52:43] Stepping pH = 7.22

Sample name: **M12_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03015**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 7:38:51 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[52:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[52:48] Stepping pH = 7.37
[53:03] Stirrer speed set to 0
[54:03] Datapoint id 50 collected
[54:03] Charge balance equation is out by -157.9%
[54:03] Stirrer speed set to 60
[54:08] pH 7.43 -> 7.63
[54:08] Using cautious pH adjust
[54:08] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:13] Stepping pH = 7.56
[54:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:18] Stepping pH = 7.60
[54:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:23] Stepping pH = 7.61
[54:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:29] Stepping pH = 7.67
[54:44] Stirrer speed set to 0
[55:44] Datapoint id 51 collected
[55:44] Charge balance equation is out by -542.8%
[55:44] Stirrer speed set to 60
[55:49] pH 7.65 -> 7.85
[55:49] Using cautious pH adjust
[55:49] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:54] Stepping pH = 7.78
[55:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:59] Stepping pH = 7.97
[56:14] Stirrer speed set to 0
[57:14] Datapoint id 52 collected
[57:14] Charge balance equation is out by -323.4%
[57:14] Stirrer speed set to 60
[57:19] pH 8.02 -> 8.22
[57:19] Using cautious pH adjust
[57:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:24] Stepping pH = 8.15
[57:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:30] Stepping pH = 8.27
[57:45] Stirrer speed set to 0
[58:45] Datapoint id 53 collected
[58:45] Charge balance equation is out by -340.7%
[58:45] Stirrer speed set to 60
[58:50] pH 8.22 -> 8.42
[58:50] Using cautious pH adjust
[58:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:55] Stepping pH = 8.29
[58:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:00] Stepping pH = 8.35
[59:00] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:05] Stepping pH = 8.51
[59:20] Stirrer speed set to 0
[59:59] Datapoint id 54 collected
[59:59] Charge balance equation is out by -425.0%
[59:59] Stirrer speed set to 60
[1:00:04] pH 8.57 -> 8.77
[1:00:04] Using cautious pH adjust
[1:00:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:09] Stepping pH = 8.60
[1:00:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:15] Stepping pH = 8.67
[1:00:15] Dispensed 0.000024 mL of Base (0.5 M KOH)



Sample name:	M12_octanol	Experiment start time:	3/3/2018 7:38:51 PM
Assay name:	pH-metric high logP	Analyst:	Pion
Assay ID:	18C-03015	Instrument ID:	T312060
Filename:	C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03015_M12_octanol_pH-metric high logP.t3r		

Experiment Log (continued)

[1:00:20] Stepping pH = 8.72
[1:00:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:25] Stepping pH = 8.80
[1:00:40] Stirrer speed set to 0
[1:01:09] Datapoint id 55 collected
[1:01:09] Charge balance equation is out by -284.9%
[1:01:09] Stirrer speed set to 60
[1:01:15] pH 8.80 -> 9.00
[1:01:15] Using cautious pH adjust
[1:01:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:20] Stepping pH = 8.81
[1:01:20] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:01:25] Stepping pH = 8.92
[1:01:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:30] Stepping pH = 8.97
[1:01:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:35] Stepping pH = 9.01
[1:01:50] Stirrer speed set to 0
[1:02:05] Datapoint id 56 collected
[1:02:05] Charge balance equation is out by -258.0%
[1:02:05] Argon flow rate set to 0
[1:02:09] Titrator arm moved over Titration position
